ASCI Simulation Development RoadMap (SDRM)

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SBSS assessment simulations are much more challenging than design of new weapons.

- Fully three dimensional geometry.
- High resolution, ~ 1 billion computational cells.
- Predictive models based on fundamental physics.
- Full-system simulations.
- Performance of aged and remanufactured weapon systems depends on microscopic material properties not previously understood or specified.

The ASCI Predictive Simulation Program has Broad Objectives.

- Performance: Create predictive simulations of nuclear weapon systems to analyze behavior and assess performance in as environment without nuclear testing.
- Safety: Predict with high certainty the behavior of full weapon systems in complex accident scenarios.
- Reliability: Achieve sufficient, validated predictive simulations to extend the lifetime of the stockpile, predict failure mechanisms, and reduce routine maintenance.
- Remanufacturing and Renewal: Use virtual prototyping and modeling to understand how new production processes and materials impact performance, safety, reliability, and aging issues.

These objectives will be realized by implementing the five ASCI strategies.

What is the RoadMap?

- The ASCI Simulation Development RoadMap (SDRM) captures the modeling issues and code features needed to support the development of simulation tools for nuclear weapon system: Performance, Safety, Aging, and Manufacturing applications.

- It provides a broad view of the modeling issues and supports planning and prioritization.

How will the RoadMap be used?

- Provide guidance to the ASCI program
  - Program scope
  - Identification of critical technical issues
  - Priorities
- Identify Relationships to Other Programs and Institutions
  - Core science program
  - Universities and major research centers
  - Experimental programs
  - Archival data

The RoadMap supports prioritization

- **Identifies critical technical issues** for the ASCI objectives: Performance, Safety, Aging, Manufacturing
  - assess the *importance* of each issue, as seen by the code users (scientists, analysts, etc.)
- **Enumerates the capabilities** (computational, theoretical, or experimental data) required to address each issue
  - assess the state of *understanding* for each capability
  - indicate the cognizant programs or institutions
- **Supports prioritization** of projects to develop needed capabilities via an *importance/understanding* matrix

The RoadMap focuses research projects and metrics

- Attention goes first toward those issues assessed most important
- Projects are defined to address important, but poorly understood phenomena
  - combinations of theoretical work, algorithm development, code implementation, or experimental data may be required
  - progress may come from ASCI or other sources
- Improvements in the state of understanding in the RoadMap provide visible metrics

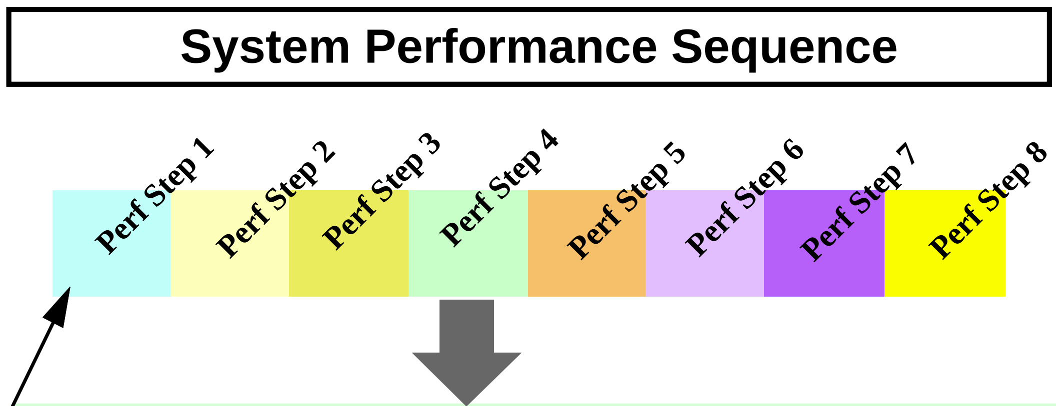
The RoadMap is aligned with the ASCI Objectives

- Performance
  - System performance sequence
- Safety
  - Abnormal environment scenarios
- Reliability (Aging)
  - Material-specific aging processes
- Reconstitution (Manufacturing)
  - Component-specific manufacturing processes

Simulation provides the only integrated SBSS testbed without additional testing…whether performance, safety, aging, or manufacturing

Simulation Development RoadMap

- Using actual stockpile issues and assessment/certification requirements, identify key simulation sequences for: Performance, Safety, Aging, and Manufacturing
- Each simulation sequence is divided into elements either by phenomenon or component
- Modeling requirements for each sequence element are included in the Simulation Development RoadMap



Performance Step 4

Issue	Impor-tance	Capability	Under-standing	Program
Phenom A	M	modeling capability X	M	ASCI
Process 1	H	modeling capability Y theoretical model input data	L M H	ASCI Science, Univ Expt program
Phenom B	M	modeling capability Z parallel algorithm archived nuc. test data	M L L	ASCI ASCI, Univ Archiving Proj
Process 2	L	theoretical model input data	H L	ASCI, Univ Expt program

Simulations Can Predict Nuclear Warhead Response in Abnormal Environments

This is essential if we are to address immediate safety and reliability problems in an aging stockpile

Safety Example

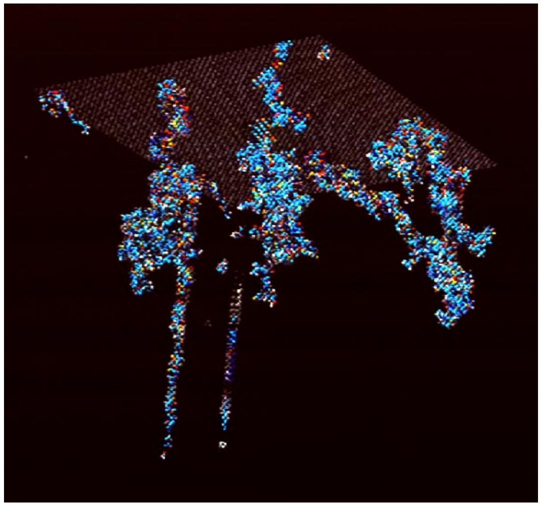
Scenario	**Critical Process**
Air Transport Accident	Shocked explosive . . .
Nearby Explosion	. . . Shocked explosive
Lightning	Shocked explosive . . .
Fire in Storage Facility	
. . more . .	

Modeling Issues
Code Features

Explosive Initiation
- Experimental Data
- Reactive Chem Modeling
  - Shock to Detonation
    - Thermal effects
    - Grain interactions
- Quantum-Atomic Material Modeling
- Phenom. Modeling
  - Void compaction

Simulation of Nuclear Component Aging is Necessary to Anticipate Performance/Safety Problems in the Stockpile

- Chemical change
  - polymer break-down, e.g., high explosive binders
  - corrosion
  - debonding and other interface effects
- Nuclear decay products
  - interstitial contamination, e.g., helium from alpha decay
  - phase stability and uniformity



Effect on Dynamic Material Properties, Tolerances and Gaps may Seriously Degrade Nuclear Performance

Aging Example

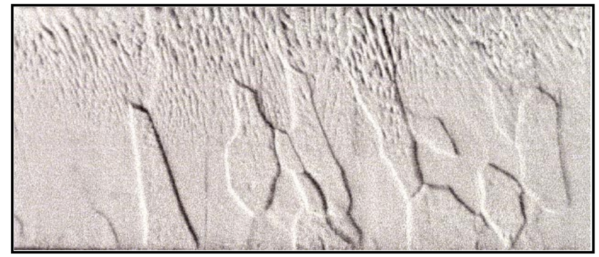
Material	**Aging Process**
Plutonium	Radiation Damage . . .
HE	. . . Radiation Damage
Polymers	Radiation Damage . . .
Solder	
. . more . .	

Modeling Issues
Code Features

Radiation Damage
- Experimental Data
- Reactive Chem Modeling
- Quantum-Atomic Material Modeling
- Phenom. Modeling
  - - Polymer
  - - HE
- Reactive Species Migration

Remanufacturing of Nuclear Components Requires New Computational Process Design

- Nuclear performance can be a sensitive function of the dynamic mechanical response of the components to high-rate/shock loading; mechanical behavior depends on microstructure of the component materials.
- Details of nuclear material structures and properties have been controlled implicitly by specifying the manufacturing process and certifying with Nuclear Testing.
- Many manufacturing processes used in stockpile warheads are no longer available or allowed. New processes must be developed quickly and they must provide tighter control of material properties and microstructures.
- New process design requires very high-end computational simulation, including state-of-the-art material science modeling.



Slow Cool

Rapid Cool

Manufacturing Example

Component

Metal parts

HE charge

Plastic components

Encapsulants

Material joins

. . more . .

Manufacturing Process

Casting

. . .

. . .

Casting

. . .

. . .

Casting

Modeling Issues

Code Features

Casting simulation

Experimental Data

Fluid Flow Modeling

Quantum-Atomic Material Modeling

Phenom. Modeling

- solidification

Microstructure evolution

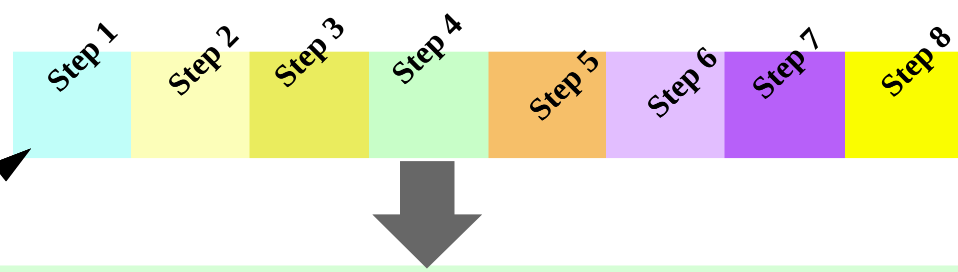
- dislocations
- grain structure

Steps to Developing a Simulation Development RoadMap

Simulation Development RoadMap

- Using the actual large-scale research problem, identify key simulation sequences
- Each simulation sequence is divided into elements, perhaps by time sequence or phenomenon
- Modeling requirements for each sequence element are included in the Simulation Development RoadMap
- Improvements to the RoadMap process are certainly possible!

Problem Sequence/Scenario/Elements



Key Step 4

Issue	Impor-tance	Capability	Under-standing	Department/ Institute
Phenom A	M	modeling capability X	M	Appl. Math
Process 1	H	modeling capability Y	L	Chemistry
		theoretical model	M	Math
		input data	H	Reactor expt
Phenom B	M	modeling capability Z	M	Physics, Eng Mechanics
		parallel algorithm	L	Comp Sci
		historical occurrence data	L	Math/Statistics
Process 2	L	theoretical model	H	Research Institute
		input data	L	Earth Sci Lab